7. *New Infrared Spectral Database Introduced to Support Remote Sensing Applications*

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Objective: To develop a "Quantitative Infrared Database" to support open-path Fourier transform (FT) infrared measurements of chemical emissions and hazardous air pollutant (HAP) molecules.

Problem: Over the last decade, growing concerns about the environment in general and air quality in particular have stimulated the development of improved, cost-effective field monitoring methods. With FT infrared-based technologies multiple airborne chemical contaminants can be measured simultaneously – because each molecular species has a unique infrared spectrum–at part-per-billion level sensitivities. The *in-situ* and real-time nature of this approach offers several advantages over traditional point source monitoring techniques for applications such as determining fugitive emissions and chemical contaminants from industrial processing plants, hazardous waste and municipal landfills, water treatment plants, oil refineries, and chemical plants. Following successful testing of FT infrared methods during remediation of several Superfund sites, the US Environmental Protection Agency (EPA) has issued a protocol (TO-16) for FT infrared open-path remote sensing. Successful implementation of this protocol is highly dependent on the availability of high-quality reference spectral data from a definitive source since molar absorptivity data in the literature widely differ.

A validated quantitative database traceable to national measurement standards is a critical part of the infrastructure required for establishing emerging infrared-based monitoring technologies. New infrared-based technologies coupled with the NIST spectral database provides both industry and EPA with a tool for assessing regulatory compliance that is both cost effective and less invasive.

Approach: SRD 79 data are based on NIST primary gravimetric standards prepared with starting materials of assessed purity and procedures that minimize contamination. For each compound, the absorption coefficient spectrum was calculated using nine transmittance spectra and the Beer's law relationship. The uncertainties in the absorption coefficient data were estimated from the linear regressions of the data and considerations of other error sources such as the non-linear detector response. For absorption coefficient values greater than 1×10^{-4} (µmol/mol) $^{-1}$ m^{-1}, the average relative uncertainty is 2.2 %. Intercomparisons with a number of expert laboratories, including the National Physical Laboratory of the UK, were used to assure the quality of the NIST data.

Results and Future Plans: Absorption coefficient data for 21 high priority HAPs on a US EPA priority list has been published as the NIST Standard Reference Database (SRD) 79, version 1.00. Data for ten additional compounds will be available shortly. The data are stored in the standard JCAMP-DX format to enable universal access to the data. The 0.12 cm^{-1} resolution data were processed to generate data at a number of different resolutions and apodizations to provide users with data that closely match their experimental parameters. A digital signature accompanies each data file, allowing users to ensure the integrity and source of the data file and traceability to NIST.

This quantitative infrared database is an ongoing project at NIST. Additional spectra will be added to the database as they are acquired and updates will be available over the Internet. Plans include continued data acquisition for the compounds listed in the 1990 US EPA Clean Air Act Amendment, as well as for those compounds that are of concern in global warming and emissions trading. Additionally, inter-comparisons of NIST primary standards and molar absorptivity data with National Metrology Institutes will be expanded to facilitate the use of this database in issues of global interest and impact.

Publications:

Chu, P.M., Guenther, F.R., Rhoderick, G.C., Lafferty, W.J., and Phillips, W.J., ***"Sample and Data Processing Considerations for the NIST Quantitative Infrared Database,"*** Proc. SPIE, 3534, 204 (1998).

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